Table 2 Stoichiometric matrix of processes and components in ASM3-ON

Process	S_O	S_I	S_S	S_{UAP}	S_{BAP}	S_{ND}	S_{NH}	S_N	S_{NO}	S_{ALK}	X_I	X_S	X_H	X_{STO}	X_A	X_{SS}	X_{ND}
1 Hydrolysis	0	f_{SI}	$1-f_{SI}$	0	0	0	$i_{N,XS}-f_{SI}\cdot i_{N,SI}-(1-f_{SI})\cdot i_{N,SS}$	0	0	$\frac{1}{14}[i_{N,XS}-f_{SI}\cdot i_{N,SI}-(1-f_{SI})\cdot i_{N,SS}]$	0	−1	0	0	0	$-i_{TS,XS}$	0
2 Aerobic storage on S_S	$Y_{STO,O}-1$	0	−1	0	0	0	$i_{N,SS}$	0	0	$\frac{1}{14}i_{N,SS}$	0	0	0	$Y_{STO,O}$	0	$0.6Y_{STO,O}$	0
2.1 Aerobic storage on UAP	$Y_{STO,O}-1$	0	0	−1	0	0	$i_{N,UAP}$	0	0	$\frac{1}{14}i_{N,UAP}$	0	0	0	$Y_{STO,O}$	0	$0.6Y_{STO,O}$	0
2.2 Aerobic storage on BAP	$Y_{STO,O}-1$	0	0	0	−1	0	$i_{N,BAP}$	0	0	$\frac{1}{14}i_{N,BAP}$	0	0	0	$Y_{STO,O}$	0	$0.6Y_{STO,O}$	0
3 Anoxic storage on S_S	0	0	−1	0	0	0	$i_{N,SS}$	$-\frac{1}{2.86}\times(Y_{STO,NO}-1)$	$\frac{1}{2.86}\times(Y_{STO,NO}-1)$	$\frac{1}{14}i_{N,SS}-\frac{1}{40.04}(Y_{STO,NO}-1)$	0	0	0	$Y_{STO,NO}$	0	$0.6Y_{STO,NO}$	0
3.1 Anoxic storage on UAP	0	0	0	−1	0	0	$i_{N,UAP}$	$-\frac{1}{2.86}\times(Y_{STO,NO}-1)$	$\frac{1}{2.86}\times(Y_{STO,NO}-1)$	$\frac{1}{14}i_{N,UAP}-\frac{1}{14}\times\frac{1}{2.86}(Y_{STO,NO}-1)$	0	0	0	$Y_{STO,NO}$	0	$0.6Y_{STO,NO}$	0
3.2 Anoxic storage on BAP	0	0	0	0	−1	0	$i_{N,BAP}$	$-\frac{1}{2.86}\times(Y_{STO,NO}-1)$	$\frac{1}{2.86}\times(Y_{STO,NO}-1)$	$\frac{1}{14}i_{N,BAP}-\frac{1}{14}\times\frac{1}{2.86}(Y_{STO,NO}-1)$	0	0	0	$Y_{STO,NO}$	0	$0.6Y_{STO,NO}$	0
4 Aerobic growth of X_H	$\frac{k_{UAP,O}+1}{1}-\frac{1}{Y_{H,O}}$	0	0	$k_{UAP,O}$	0	0	$-i_{N,BM}-k_{UAP,O}-i_{N,UAP}$	0	0	$\frac{1}{14}(-i_{N,BM}-k_{UAP,O}\cdot i_{N,UAP})$	0	0	1	$-1/Y_{H,O}$	0	$i_{TS,BM}-\frac{0.6}{Y_{H,O}}$	0

Table 2 Stoichiometric matrix of processes and components in ASM3-ON

Process	S_O	S_I	S_S	S_{UAP}	S_{BAP}	S_{ND}	S_{NH}	S_N	S_{NO}	S_{ALK}	X_I	X_S	X_H	X_{STO}	X_A	X_{SS}	X_{ND}
5 Anoxic growth of X_H	0	0	0	$k_{UAP,NO}$	0	0	$-i_{N,BM}-k_{UAP,NO}\cdot i_{N,UAP}$	$-\frac{1}{2.86}\times(k_{UAP,NO}+1-\frac{1}{Y_{H,NO}})$	$\frac{1}{2.86}\times(k_{UAP,NO}+1-\frac{1}{Y_{H,NO}})$	$\frac{1}{14}\left(-i_{N,BM}-k_{UAP,NO}\cdot i_{N,UAP}\right)-\frac{1}{40.04}(k_{UAP,NO}+1-\frac{1}{Y_{H,NO}})$	0	0	1	$-1/Y_{H,NO}$	0	$i_{TS,BM}-\frac{0.6}{Y_{H,NO}}$	0
6 Aerobic endogenous respiration of X_H	$k_{BAP,O}+f_I-1$	0	0	0	$k_{BAP,O}$	0	$i_{N,BM}-f_I\cdot i_{N,XI}-k_{BAP,O}\cdot i_{N,BAP}$	0	0	$\frac{1}{14}(i_{N,BM}-f_I\cdot i_{N,XI}-k_{BAP,O}\cdot i_{N,BAP})$	f_I	0	−1	0	0	$f_I\cdot i_{TS,XI}-i_{TS,BM}$	0
7 Anoxic endogenous respiration of X_H	0	0	0	0	$k_{BAP,NO}$	0	$i_{N,BM}-f_I\cdot i_{N,XI}-k_{BAP,NO}\cdot i_{N,BAP}$	$-\frac{1}{2.86}\times(k_{BAP,NO}+f_I-1)$	$\frac{1}{2.86}\times(k_{BAP,NO}+f_I-1)$	$\frac{1}{14}[i_{N,BM}-f_I\cdot i_{N,XI}-k_{BAP,NO}\cdot i_{N,BAP}-\frac{1}{2.86}(k_{BAP,NO}+f_I-1)]$	f_I	0	−1	0	0	$f_I\cdot i_{TS,XI}-i_{TS,BM}$	0
8 Aerobic growth on X_{STO}	–1	0	0	0	0	0	0	0	0	0	0	0	0	–1	0	–0.6	0
9 Anoxic growth on X_{STO}	0	0	0	0	0	0	0	$\frac{1}{2.86}$	$-\frac{1}{2.86}$	$\frac{1}{40.04}$	0	0	0	–1	0	–0.6	0
10 Aerobic growth of X_A	$\frac{k_{UAPO,O}}{-\frac{4.57}{Y_A}+1}$	0	0	$k_{UAPA,O}$	0	0	$-k_{UAPA,O}\cdot i_{N,UAP}-\frac{1}{Y_A}-i_{N,BM}$	0	$1/Y_A$	$\frac{1}{14}(-k_{UAPA,O}\cdot i_{N,UAP}-\frac{2}{Y_A}-i_{N,BM})$	0	0	0	0	1	$i_{TS,BM}$	0

Table 2 Stoichiometric matrix of processes and components in ASM3-ON

Process	S_O	S_I	S_S	S_{UAP}	S_{BAP}	S_{ND}	S_{NH}	S_N	S_{NO}	S_{ALK}	X_I	X_S	X_H	X_{STO}	X_A	X_{SS}	X_{ND}
11 Aerobic endogenous respiration of X_A	$k_{BAPA,O}+f_I-1$	0	0	0	$k_{BAPA,O}$	0	$i_{N,BM}-k_{BAPA,O}\cdot i_{N,BAP}-f_I\cdot i_{N,XI}$	0	0	$\frac{1}{14}(i_{N,BM}-k_{BAPA,O}\cdot i_{N,BAP}-f_I\cdot i_{N,XI})$	f_I	0	0	0	−1	$f_I\cdot i_{TS,XI}-i_{TS,BM}$	0
12 Anoxic endogenous respiration of X_A	0	0	0	0	$k_{BAPA,NO}$	0	$i_{N,BM}-k_{BAPA,NO}\cdot i_{N,BAP}-f_I\cdot i_{N,XI}$	$-\frac{1}{2.86}\times(k_{BAPA,NO}+f_I-1)$	$\frac{1}{2.86}\times(k_{BAPA,NO}+f_I-1)$	$\frac{1}{14}[i_{N,BM}-k_{BAPA,NO}\cdot i_{N,BAP}-f_I\cdot i_{N,XI}-\frac{1}{2.86}(k_{BAPA,NO}+f_I-1)]$	f_I	0	0	0	−1	$f_I\cdot i_{TS,XI}-i_{TS,BM}$	0
13 Ammonification of DON	0	0	0	0	0	–1	1	0	0	1/14	0	0	0	0	0	1	0
14 Hydrolysis of entrapped ON	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	–1	−1